DFT-NEGF calculations of gated graphene nano-structures

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DFT-NEGF calculations of gated graphene nano-structures

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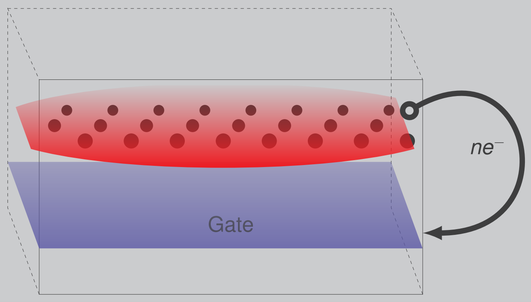
Abstract

Two dimensional (2D) materials such as graphene are expected to be prominent candidates for nanoscale electronics applications. In particular the possibility to electrostatically gate 2D atomic scale structures is a key feature. Here we present non-equilibrium simulations of graphene nanostructures to illustrate a novel electrostatic gating implementation in SIESTA [1].
We test this model on a graphene nanoconstriction and investigate the doping and the applied bias dependence on the transmission.

Implementation details

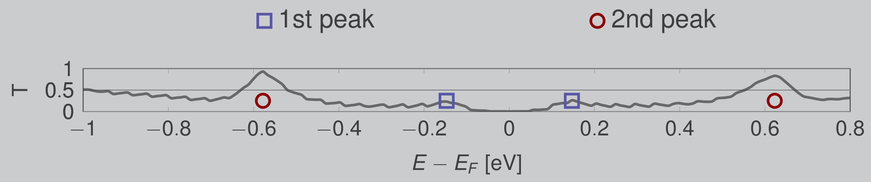


- Different gate geometries possible
- 2D materials only
- Electric field obtained from Poisson
- Self-consistent solution in SIESTA [1]

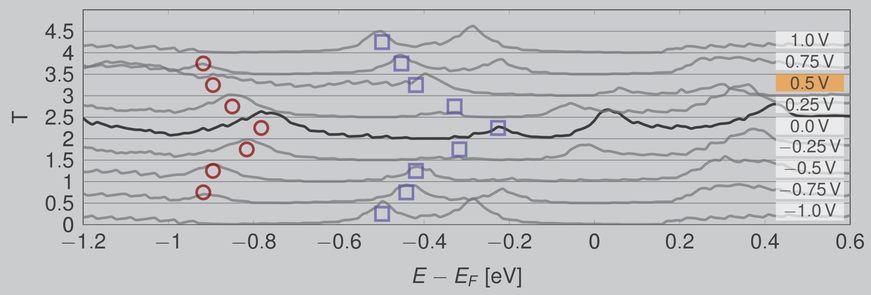
Colour convention: $+e^-$ $-e^-$

Transmission properties of gating nanoconstriction [2]

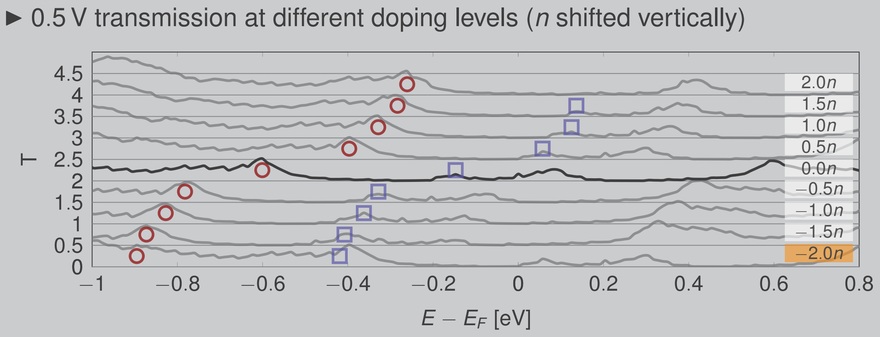
- Intrinsic transmission at 0 V



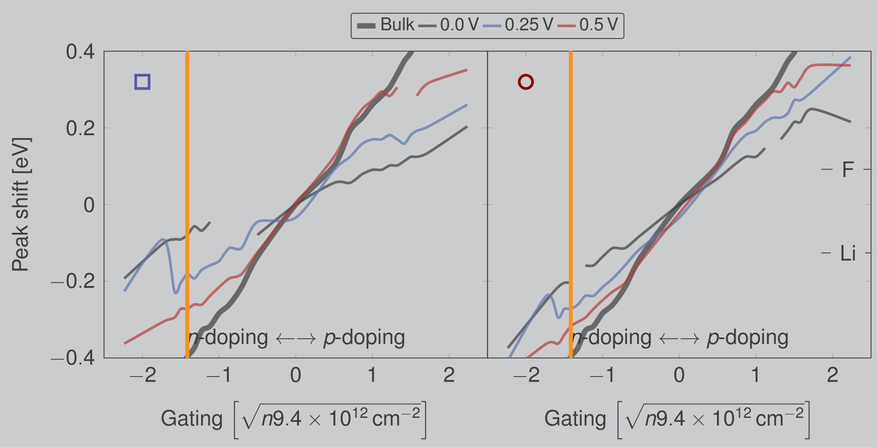
- $n = -2.0e^-$ transmission at different applied bias (V shifted vertically), symmetric about applied bias



- 0.5 V transmission at different doping levels (n shifted vertically)



- Transmission peak doping compared to graphene doping

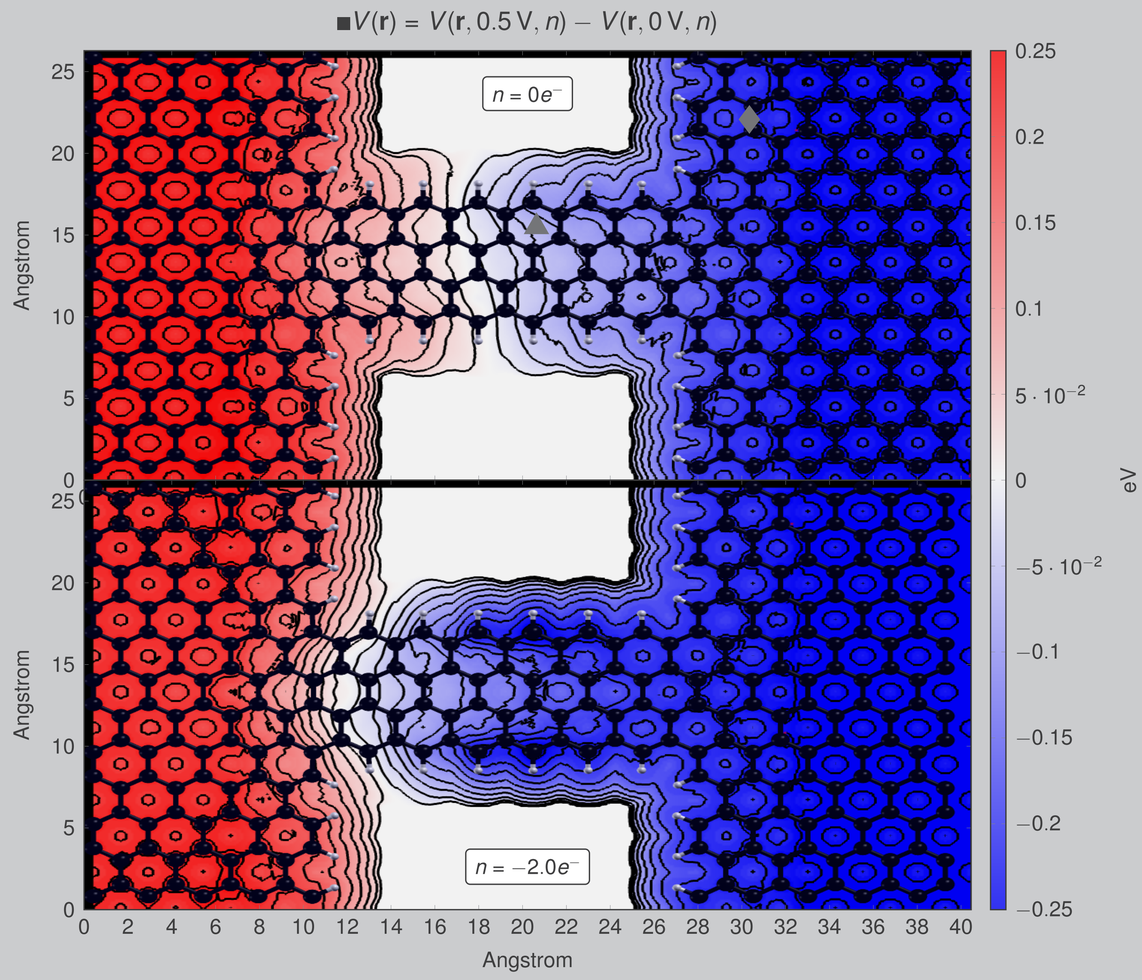


- Gating nanoconstriction does not follow linear $\sqrt{n}$ dependence
- Transmission peak position dependent on applied bias and doping

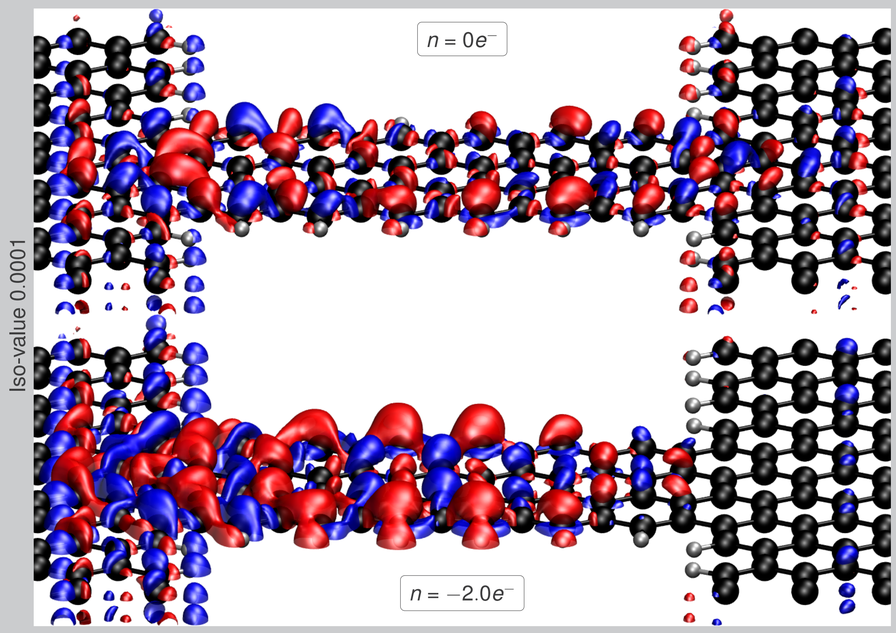
Explicit doping and bias analysis

Analysis of 0.5 V and $n = -2.0e^-$

- Electrostatic potential tuned by doping



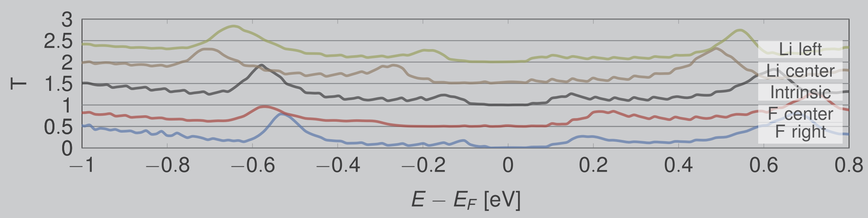
- Charge redistribution is consistent with the doping effect of the electrostatic potential



- Gating nanoconstriction shifts potential drop to one end
- Possible enhancement of reactivity at localised potential drop

Doping via adsorbates

- Doping with Fluor and Lithium in positions
  - ▲ Center adsorption
  - ♦ Adsorption outside of constriction



We examine the effect of a donor Li or acceptor F adatom either inside the constriction, at the center position (CP), or outside (OP); see example positions in the potential plot.
The Li and F atoms are positioned above the center of a hexagon or ontop a carbon atom, respectively.
The transmission plot indicates that there is no significant scattering (except for the hole peaks in the case where F is at CP).
From the most significant peak shift we find that Li donates at least 0.2 electrons to graphene while F accepts at least 0.3 electrons from graphene, from looking at the bulk doping profile.
In addition, most of the doping effect is still present if the adatoms are moved outside the constriction.

Conclusion

- New electrostatic gating model implemented for SIESTA/TranSIESTA
- Investigating the model on a graphene nanoconstriction
  - Gating is not the same as shifting Fermi-level
  - Features of transmission spectra does not shift linearly with $\sqrt{n}$
  - Electronic structure can be tuned via doping
  - Potential drop across constriction changes with doping, we can therefore tune the local potential drop by gating
- Localised potential drop could influence the reactivity
- Gating other graphene nanostructures could also show non-linear effects
- Currently investigating oxygen terminated nanoconstriction

[1] J. M. Soler *et al. Journal of Physics: Condensed Matter* 14.11 (Mar. 2002).
[2] T. Gunst *et al.* (May 2013). arXiv: 1305.5907.
[3] M. Brandbyge *et al. Physical Review B* 65.16 (Mar. 2002).
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